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The phase-dependent linear conductance of a superconducting quantum point contact

A Levy Yeyati, A Martín-Rodero and J C Cuevas

Departamento de Física de la Materia Condensada C-XII, Facultad de Ciencias, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

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Abstract. The exact expression for the phase-dependent linear conductance of a weakly damped superconducting quantum point contact is obtained. The calculation is performed by summing the complete perturbative series in the coupling between the electrodes, thus taking into account all possible multiple Andreev reflections inside the gap. The failure of any finite-order perturbative expansion in the limit of small voltage and small quasiparticle damping is analysed in detail. In the low-transmission regime this nonperturbative calculation yields a result which is at variance with standard tunnel theory. Our result exhibits an unusual phase dependence at low temperatures in qualitative agreement with the available experimental data.

In the last few years there has been renewed interest in the theory of superconducting weak links associated with the increasing technological capability for the fabrication of nanoscale superconducting devices. This opens up the possibility for a closer comparison between theoretical models and clean experiments involving a few quantum conducting channels [1]. On the theoretical side and especially since the work of Klapwijk *et al* [2], the crucial role played by multiple Andreev reflections (MAR) in the transport properties of superconducting contacts has become well established. However, quantitative results for the small-bias regime are difficult to obtain due to the increasing number of MAR taking place within the subgap region for decreasing voltages [3]. A more complete theoretical description of the stationary and nonstationary transport properties of superconducting contacts with arbitrary transparency at small bias voltages is therefore desirable. In this direction, there have been a number of recent studies analysing the transport properties of a single-channel superconducting quantum point contact (SQPC) [4].

In this paper we present a theoretical approach for the calculation of the dc and ac currents of an SQPC for arbitrary values of the contact transparency, bias voltage and temperature. We shall concentrate on the limit $V/\Delta \to 0$ for which we obtain an exact analytical expression of the total current. The nondissipative part of this current agrees with previously known results in both the tunnel and the ballistic regimes. From the dissipative part we extract an expression for the phase-dependent linear conductance which, in the limit of small barrier transparency, differs from the standard tunnel theory result and is consistent with the available experimental data.

We consider a short weak link as represented schematically in figure 1. It consists of two wide electrodes connected by a narrow constriction of length L_c much smaller than the superconducting coherence length ξ_0, and having a width comparable to the Fermi wavelength λ_F. For simplicity we shall consider the case of a single quantum conducting channel. In previous work we have analysed the dc transport properties of such

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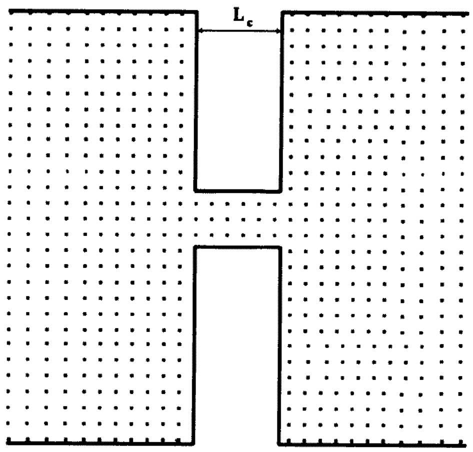

Figure 1. Schematic representation of our discretized point contact model.

a system by solving self-consistently the Bogoliubov–de Gennes equations written in a local representation [5]. These equations can be derived from a Hamiltonian having the form [5]

$$\hat{H} = \sum_{i,\sigma} (\epsilon_i - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_{i \neq j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} (\Delta^*_i c^{\dagger}_{i\downarrow} c^{\dagger}_{i\uparrow} + \Delta_i c_{i\uparrow} c_{i\downarrow}) \tag{1}$$

where the indexes i and j run over the discrete sites describing the system. As shown in [5] for the case of a short weak link ($L_c \ll \xi_0$) the self-consistent order parameter profile can be well approximated by a step function. Thus for a symmetrical contact we have $|\Delta_L| = |\Delta_R| = \Delta$ and $\phi = \phi_L - \phi_R$, where Δ is the gap parameter, ϕ_L and ϕ_R being the superconducting phases on each of the electrodes.

Under these conditions and in the presence of an applied bias voltage $eV = \mu_L - \mu_R$, the system dynamics can be studied by analysing the following time-dependent Hamiltonian:

$$\hat{H}(\tau) = \hat{H}_L + \hat{H}_R + \sum_{\sigma} (t \mathrm{e}^{\mathrm{i}\phi(\tau)/2} c^{\dagger}_{L\sigma} c_{R\sigma} + t \mathrm{e}^{-\mathrm{i}\phi(\tau)/2} c^{\dagger}_{R\sigma} c_{L\sigma}) \tag{2}$$

where H_L and H_R describe the regions where the order parameter is homogeneous while the hopping term describes the charge transfer through the quantum channel coupling the two electrodes. The coupling parameter t fixes the normal-transmission coefficient of the contact [6] and $\phi(\tau) = \phi_0 + 2eV\tau/\hbar$. Notice that within this representation the time-dependent phase only appears in the phase factors multiplying the hopping elements [7].

We would like to emphasize that starting from this simple contact model a unified description of N–N [6], N–S [8] and S–S [5] contacts can be obtained. The definition of the normal-transmission coefficient α in terms of the microscopic parameters of the model allows us to establish a complete correspondence with the scattering approach [9].

The transport properties of this model can be analysed using nonequilibrium Green functions technique [3, 5, 10] with the time-dependent coupling term treated as a perturbation. The most relevant quantity in this formalism is the nonequilibrium distribution function $G^{+,-}$, which in a superconducting broken-symmetry (Nambu) representation is defined by

$$\hat{G}^{+-}_{i,j}(\tau,\tau') = \mathrm{i} \begin{pmatrix} \langle c^{\dagger}_{j\uparrow}(\tau') c_{i\uparrow}(\tau) \rangle & \langle c_{j\downarrow}(\tau') c_{i\uparrow}(\tau) \rangle \\ \langle c^{\dagger}_{j\uparrow}(\tau') c^{\dagger}_{i\downarrow}(\tau) \rangle & \langle c_{j\downarrow}(\tau') c^{\dagger}_{i\downarrow}(\tau) \rangle \end{pmatrix}.$$

In terms of these functions the current through the contact can be written as

$$I(\tau) = \frac{2e}{\hbar}\left[\hat{t}(\tau)\hat{G}^{+-}_{RL}(\tau,\tau) - \hat{t}^{\dagger}(\tau)\hat{G}^{+-}_{LR}(\tau,\tau)\right]_{11} \tag{3}$$

where $\hat{t}$ is the matrix hopping element in the Nambu representation

$$\hat{t} = \begin{pmatrix} t\mathrm{e}^{\mathrm{i}\phi(\tau)/2} & 0 \\ 0 & -t\mathrm{e}^{-\mathrm{i}\phi(\tau)/2} \end{pmatrix}. \tag{4}$$

Within this perturbative approach the standard tunnel theory expression for the current $I = I_J \sin\phi + G_0(1 + \epsilon\cos\phi)V$ [11] can be obtained to the lowest order in t. The conductance $G(\phi) = G_0(1+\epsilon\cos\phi)$ thus obtained becomes a divergent quantity in the limit $V \to 0$ [12]. In order to ensure the existence of a linear regime, a finite-energy relaxation rate η must be introduced into this superconducting mean-field theory (η represents the damping of the quasiparticle states, which in a real system is always present due to inelastic scattering processes). As we shall see, according to the value of η and the normal-transmission coefficient α, two different regimes can be identified: the weakly damped regime, for which $\eta \ll \alpha\Delta$, and the strongly damped case, where $\eta \gg \alpha\Delta$. In this work we are mostly concerned with the analysis of the first regime, where the most interesting effects appear.

A remarkable fact about the perturbative expansion in the weakly damped situation is that contributions corresponding to higher-order processes turn out to be increasingly divergent in the zero-bias limit [13]. In particular, it can be easily demonstrated that contributions to the total current of order t^{2n}, $n \geqslant 2$, diverge like $\sim t^{2n}/\eta^{n-1}$ (the lowest-order contribution diverges as $\sim t^2 \ln\eta$). This result is a direct consequence of the increasing contribution from the superconducting gap edge singularities. Therefore, a correct answer cannot be found in principle by means of a finite-order perturbative expansion. This fact has been usually considered as the main drawback of the Hamiltonian approach [14].

One could draw a formal analogy with the case of a high-density electron gas, where the diagrammatic expansion in the bare Coulomb potential is also increasingly divergent. As in that case, the solution can be found by 'dressing' the perturbative potential, i.e. $\hat{t}$. In the present problem the dressed quantities (left–right coupling, propagators) can be exactly obtained in the zero-voltage limit by evaluating the complete perturbative series. To this end, we find it convenient to express all quantities in terms of a renormalized left–right coupling element which satisfies the following Dyson equation:

$$\hat{T}^{a,r}(\tau,\tau') = \hat{t}(\tau)\,\delta(\tau-\tau') + \hat{t}(\tau)\hat{g}^{a,r}_{R}(\tau-\tau_1)\hat{t}^{\dagger}(\tau_1)\hat{g}^{a,r}_{L}(\tau_1-\tau_2)\hat{T}^{a,r}(\tau_2,\tau') \tag{5}$$

where $\hat{g}^{a,r}_{L}$ and $\hat{g}^{a,r}_{R}$ represent the (advanced, retarded) Green functions of the uncoupled left and right electrodes respectively (integration over internal times is implicitly assumed). From equation (5), the relation between the renormalized coupling $\hat{T}$ and the exact (advanced and retarded) Green functions is easy to obtain. In the same way, the nonequilibrium distribution function $\hat{G}^{+-}$, which is related to $\hat{G}^{r}$ and $\hat{G}^{a}$, can be written in terms of $\hat{T}$ [15].

Integral equations like equation (5) adopt a simpler form when Fourier transformed with respect to their temporal arguments [3, 15]. Defining the Fourier components $\hat{T}_{n,m}(\omega)$ as

$$\hat{T}_{n,m} = \int \mathrm{d}\tau \int \mathrm{d}\tau'\ \mathrm{e}^{-\mathrm{i}\left(n\phi(\tau)-m\phi(\tau')\right)/2}\,\mathrm{e}^{-\mathrm{i}\omega(\tau-\tau')}\hat{T}(\tau,\tau') \tag{6}$$

the total current can be expressed in the form

$$I(\tau) = \sum_m I_m \exp \mathrm{i}m\phi(\tau)/2$$

where the complex coefficients, I_m, do not depend on $\phi(\tau)$ and are given by

$$I_m = \frac{2e}{h}\int \mathrm{d}\omega \sum_n \Big[\hat{T}^r_{0,n}\hat{g}^{+-}_{R_{n,n}}\hat{T}^{r\dagger}_{n,m}\hat{g}^a_{L_{m,m}} - \hat{g}^r_{L_{0,0}}\hat{T}^r_{0,n}\hat{g}^{+-}_{R_{n,n}}\hat{T}^{r\dagger}_{n,m} + \hat{g}^r_{R_{0,0}}\hat{T}^{a\dagger}_{0,n}\hat{g}^{+-}_{L_{n,n}}\hat{T}^a_{n,m} - \hat{T}^{a\dagger}_{0,n}\hat{g}^{+-}_{L_{n,n}}\hat{T}^a_{n,m}\hat{g}^a_{R_{m,m}}\Big]_{11}. \tag{7}$$

It can be seen from equation (5) that $\hat{T}_{n,m} = 0$ for even $n - m$ and therefore only even Fourier components of the current are different from zero. The components $\hat{T}_{n,n+m}$ correspond to processes where at least $(|m| - 1)/2$ Andreev reflections are involved.

For the following analysis it is useful to decompose the total current into dissipative and nondissipative contributions. The supercurrent part, given by

$$I_S = -2\sum_{m>0} \mathrm{Im}(I_m)\sin[m\phi(\tau)]$$

tends to a finite value in the limit $V \to 0$. On the other hand, the dissipative part is given by

$$I_D = I_0 + 2\sum_{m>0} \mathrm{Re}(I_m)\cos[m\phi(\tau)]$$

and goes to zero as $I_D \sim G(\phi)V$, $G(\phi)$ being the zero-voltage conductance. The linear term can be straightforwardly derived from equation (7) by expanding the Fermi functions appearing in $\hat{g}^{+-}_{L,R}$ [16] up to first order in V and evaluating the remaining factors at zero voltage.

In this limit the Fourier components satisfy $\hat{T}_{n,m} = \hat{T}_{0,m-n} \equiv \hat{T}_{m-n}$, and can be shown to obey the simple recursive relations

$$\begin{aligned}&\hat{T}_{n+2}(\omega) = z(w)\hat{T}_n(\omega)\\ &\hat{T}_{-n-2}(\omega) = z(\omega)\hat{T}_{-n}(\omega) \qquad (n \geqslant 1)\end{aligned} \tag{8}$$

where $z(\omega)$ is a scalar complex function generating an extra Andreev reflection. In the weakly damped regime and within the energy interval $\Delta > |\omega| > \Delta\sqrt{1-\alpha}$ this function reduces to a phase factor $z(\omega) = \exp \mathrm{i}\varphi(\omega)$, where

$$\varphi(\omega) = \arcsin\left(\frac{2}{\alpha\Delta^2}\sqrt{\Delta^2 - \omega^2}\sqrt{\omega^2 - (1-\alpha)\Delta^2}\right). \tag{9}$$

This clearly shows that within this energy interval all multiple-scattering processes (which correspond to MAR) become equally important. Therefore, all Fourier components contribute to the renormalized coupling in this region, giving rise to singularities which are associated with the existence of interface bound states. In fact, the renormalized coupling in this energy region can be easily obtained from equations (8) and (9), giving

$$\sum_n \hat{T}_n \mathrm{e}^{\mathrm{i}n\phi/2} = \frac{\hat{T}_1 \mathrm{e}^{\mathrm{i}\phi/2}\mathrm{e}^{\mathrm{i}(\varphi+\phi)}}{1 - \mathrm{e}^{\mathrm{i}(\varphi+\phi)}} + \frac{\hat{T}_{-1}\mathrm{e}^{-\mathrm{i}\phi/2}\mathrm{e}^{\mathrm{i}(\varphi-\phi)}}{1 - \mathrm{e}^{\mathrm{i}(\varphi-\phi)}}$$

which exhibits singularities at $\varphi(\omega) = \pm\phi$. From equation (9) it follows that these singularities correspond to simple poles at

$$\omega_S = \pm\Delta\sqrt{1 - \alpha\sin^2(\phi/2)}.$$

These are the interface bound states inside the gap of a superconducting point contact, as derived by different authors [17, 18].

In the same way, the complete harmonic series must be evaluated in order to obtain the contributions to both the dissipative and the nondissipative parts of the current coming from the energy range $\Delta > |\omega| > \Delta\sqrt{1-\alpha}$. Again, these infinite summations can be easily performed making use of the recursive relations of equation (8). It is then found that the integrand for both parts of the current becomes singular at $\omega = \pm\omega_S$. The contribution of these poles yields

$$I_S(\phi) = \frac{e\Delta}{2\hbar} \frac{\alpha \sin\phi}{\sqrt{1-\alpha\sin^2(\phi/2)}} \tanh\left(\frac{\beta\omega_S}{2}\right) \tag{10}$$

and

$$I_D(\phi) = \frac{2e^2}{h} \frac{\pi}{16\eta} \left[\frac{\Delta\alpha\sin\phi}{\sqrt{1-\alpha\sin^2(\phi/2)}} \operatorname{sech}\left(\frac{\beta\omega_S}{2}\right)\right]^2 \beta V. \tag{11}$$

In equation (10) the previously known result for the zero-bias supercurrent is recovered [19, 5]. This expression interpolates between the Ambegaokar–Baratoff result for the tunnel limit [20] and the Kulik–Omel'yanchuk one for the ballistic ($\alpha \to 1$) regime [17].

The expression for the dissipative current given above is the main result of this work. The linear conductance thus obtained depends on η as $\sim 1/\eta$, i.e. is proportional to the number of MAR taking place before the quasiparticles are inelastically scattered (roughly given by $\alpha\Delta/\eta$). This means that for a weakly damped contact MAR dominates over single-quasiparticle tunnelling [21]. This is also reflected in the α^2-dependence of equation (11).

Our theory yields a phase-dependent linear conductance which strongly deviates from the tunnel theory result. In the limit of low barrier transparency, equation (11) predicts $G(\phi) \sim 1 - \cos(2\phi)$ instead of the form $G(\phi) \sim 1 + \epsilon\cos\phi$ of standard tunnel theory. Therefore, the tunnel theory linear conductance can never be recovered in the weakly damped regime. On the other hand, with increasing values of η MAR are progressively damped (the function $z(\omega)$ is no longer a phase factor, decaying exponentially with η); eventually, when $\eta \gg \alpha\Delta$ only the lowest-order processes contribute to the current and the tunnel theory expression is recovered. Figures 2(a) and 2(b) illustrate in an explicit way the transition from the weakly to the strongly damped regimes, allowing one to establish precisely the range of validity of our equation (11) for $G(\phi)$. In figure 2(a) the ratio between the exact linear conductance, obtained by solving equations (5) and (7) numerically, and the analytical expression for equation (11), are plotted as functions of η/Δ for increasing values of α. As can be observed, this ratio tends to unity for η/Δ sufficiently small, within the range where $\eta < \alpha\Delta$. On the other hand, the validity of standard tunnel theory in the strongly damped regime is illustrated in figure 2(b), where the ratio between the exact numerical conductance and the tunnel theory ($\mathrm{O}(t^2)$) conductance is represented against η/Δ. From this figure it is clear that tunnel theory becomes valid only for sufficiently small α, provided that $\alpha \ll \eta/\Delta$. In a real contact, where the inelastic scattering rate η can be expected to be a small fraction of Δ, our expression for $G(\phi)$ will be valid provided that the transparency is not extremely low.

It is worth mentioning that the strong sensitivity of the dissipative current to a phenomenological inelastic scattering rate was pointed out by several authors during the 1970s. This fact was used for trying to reach an agreement between the standard tunnel theory conductance and the experimental results (for a review on the discrepancy between standard tunnel theory and experiments, usually referred to as the '$\cos(\phi)$-problem', see [12] and [22]). However, as shown above, when the condition $\eta < \alpha\Delta$ holds, the standard tunnel theory can *never* give the correct result.

Another interesting limiting case of equation (11) corresponds to the ballistic regime. In this case and for $T \sim T_C$, $G(\phi)$ behaves approximately as $1 - \cos\phi$, in agreement with the result given by Zaitsev [10]. However, the most unusual phase dependence of $G(\phi)$ appears

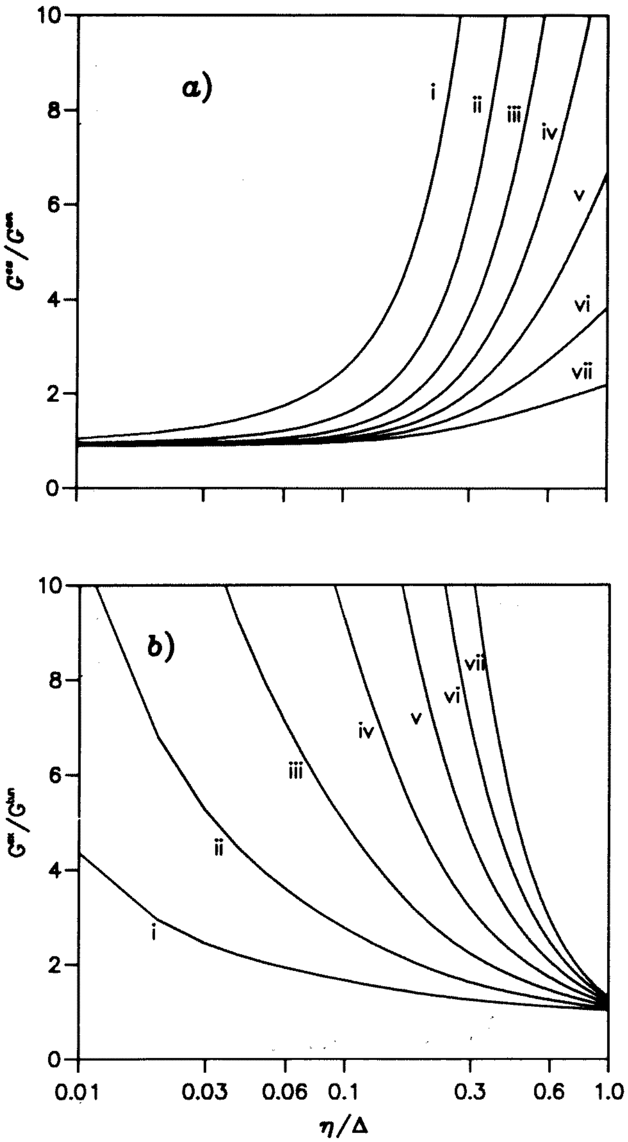

Figure 2. The transition between the weakly and strongly damped regimes. The ratio between the exact numerical conductance and: (a) the analytical expression given in equation (11); and (b) the tunnel theory ($O(t^2)$) conductance, plotted against η/Δ. The values of α considered are (i) 0.15, (ii) 0.48, (iii) 0.64, (iv) 0.78, (v) 0.88, (vi) 0.95 and (vii) 0.99. In all cases the phase is the one corresponding to the maximum supercurrent.

for high values of the transmission and low temperatures ($k_B T < \Delta$). This is illustrated in figure 3, where $G(\phi)$ is plotted for two different temperatures and increasing values of the transmission.

The only experiment where the full phase dependence of $G(\phi)$ was measured, as far as we know, is that of [23]. Their measured $G(\phi)$ strongly deviates from a $\cos\phi$-like form, being almost negligible for small values of ϕ and exhibiting a large increase at around

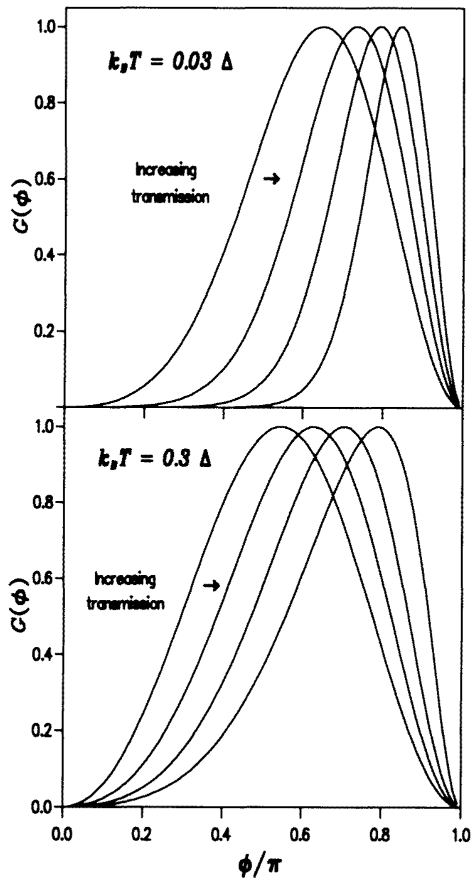

Figure 3. The phase dependence of the linear conductance given by equation (11) for two different temperatures and increasing values of the normal-transmission coefficient ($G(\phi)$ is normalized to its maximum value).

$\phi \sim \pi/2$. As can be observed in figure 3, this behaviour is in qualitative agreement with our results for sufficiently large transmission. However, a detailed comparison would require a more exhaustive experimental study of $G(\phi)$ for different barrier transparencies and temperature regimes. We believe that these measurements are now becoming feasible with recent advances in the fabrication of nanoscale superconducting contacts [1].

In conclusion, it has been shown that a nonperturbative calculation is needed for obtaining the total current through a weakly damped superconducting point contact in the linear regime. Using a simple model Hamiltonian we are able to obtain exactly the phase-dependent linear conductance. The resulting expression is in good agreement with the available experimental data and we believe that it can provide motivation for more detailed experimental studies.

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